TECHNISCHE UNIVERSITÄT
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Björn Sprungk
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Research Group Uncertainty Quantification

Sensitivity of uncertainty quantification and Bayesian inverse problems

Joint work with Oliver Ernst and Alois Pichler (TU Chemnitz)

June 8th, 2022

GDR MASCOT-NUM Annual Meeting, Clermont Ferrand

Outline

1. Uncertainty Propagation
2. Risk Functionals
3. Bayesian Inversion

Random Partial Differential Equations

- Consider general PDE with solution $u \in \mathscr{U}$ and coefficient(s) $a \in \mathscr{A}$ given by

$$\mathscr{F}(u, a) = 0$$

- **Running example**: Elliptic diffusion equation on compact $D \subseteq \mathbb{R}^2$,

$$-\nabla \cdot (\mathrm{e}^{a} \nabla u) = f, \qquad u\big|_{\partial D} \equiv 0$$

with $\mathscr{U} = H_0^1(D)$ and $\mathscr{A} = L^\infty(D)$ (weak form)

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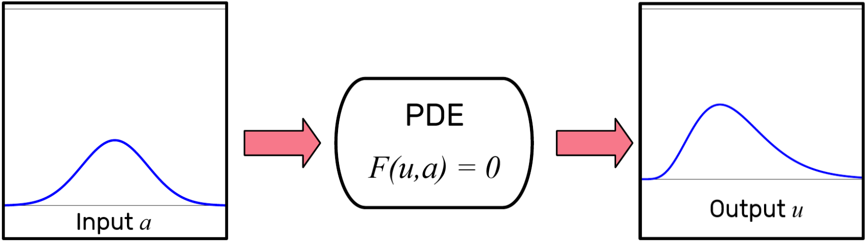
- **UQ approach:**
  1. Describe uncertainty about a by probability measure μ on $\mathscr{A}$
  2. Compute resulting probability distribution ν on $\mathscr{U}$ of random solution u or quantity of interest $q(u)$ where $q\colon \mathscr{U} \to \mathbb{R}$

UQ Scheme



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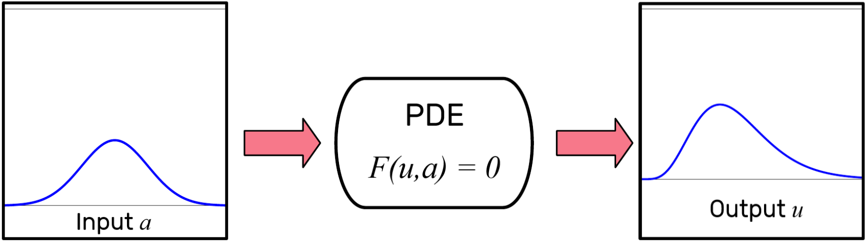

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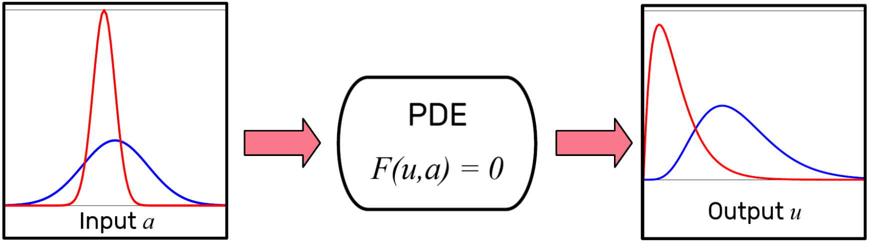

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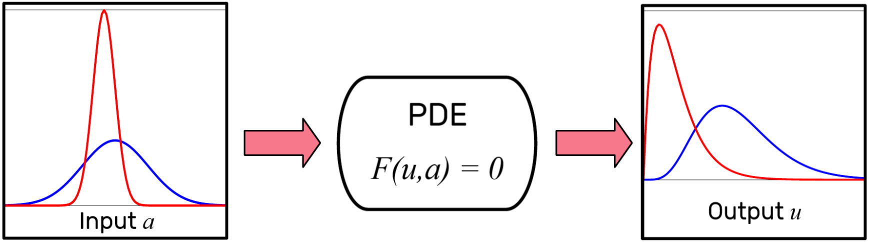

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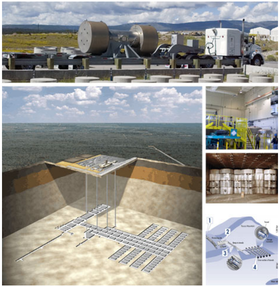
Question

Can we control the effect of perturbations of μ on output distribution ν?

Motivational Example



source: Sandia National Labs

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- Computational model given by PDE

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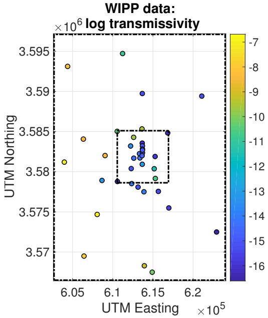

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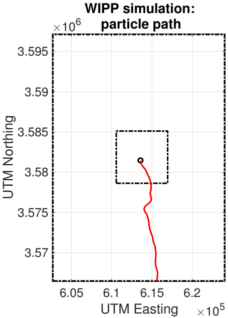

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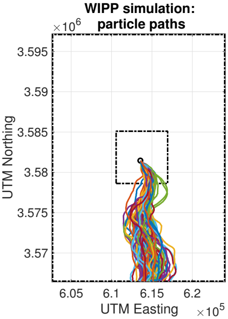

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UQ approach:

1. Model uncertain spatially varying log conductivity a by Gaussian process
2. Use available data to estimate stochastic model for a
3. Compute resulting distribution of exit times q_{exit}

Gaussian random fields

- We assume $a \sim \mathsf{N}(m, c)$ with mean and covariance function m and c

$$\begin{aligned} \mathsf{E}\left[a(x)\right] &= m(x), \\ \mathsf{Cov}[a(x), a(y)] &= c(x, y), \\ a(x) &\sim \mathsf{N}\left(m(x), c(x, x)\right) \end{aligned}$$

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- Common parametrized class: Matérn covariance functions

$$c_{\sigma^2,\rho,k+\frac{1}{2}}(x,y) := \sigma^2 \ \mathrm{e}^{-\frac{\sqrt{2k+1}}{\rho}|x-y|} \ P_k\left(\frac{\sqrt{2k+1}}{\rho}|x-y|\right)$$

with variance $\sigma^2 > 0$, correlation length $\rho > 0$, smoothness $k + \frac{1}{2}$, $k \in \mathbb{N}_0$

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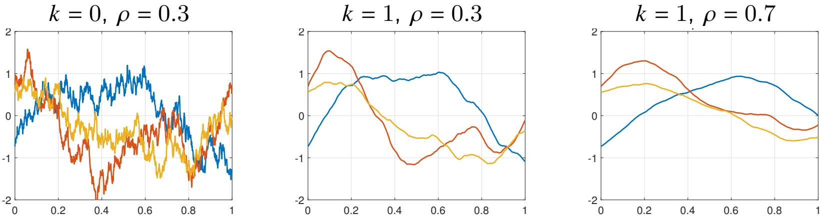

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- In practice, we obtain estimates $\widehat{\sigma}^2$, $\widehat{\nu}$, $\widehat{\rho}$ of the parameters given observational data $a(x_j)$, $j = 1, \ldots, n$ (e.g., by maximum-likelihood)

Motivational Question

How does estimation error or different choice of parameters, e.g., for σ^2, affect the output of the UQ analysis?

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- **Running example:** For elliptic problem $-\nabla \cdot (\mathrm{e}^{a} \nabla u) = f$ we have

$$\|u - \widehat{u}\|_{H_0^1(D)} = \|S(a) - S(\widehat{a})\|_{H_0^1(D)} \;\leq\; c_f \, \mathrm{e}^{3r} \;\; \|a - \widehat{a}\|_{L^\infty(D)}$$

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- Does Lipschitz continuity of S yield Lipschitz continuity of $\mu \mapsto S_*\mu$?

Sensitivity in TV Distance

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- **But:** TV distance not suited for measures on infinite-dimensional spaces, e.g., for Gaussian measures associated to Gaussian processes we have

$$d_{\mathsf{TV}}\left(\mathsf{N}(m, C), \mathsf{N}(m, \sigma^2 C)\right) = 1 \qquad \text{if } \sigma \neq 1,$$

i.e., any estimation error in variance parameter σ^2 yields maximal distance

Wasserstein Distance

- Instead, we consider the p-Wasserstein distance

$$\mathsf{W}_p(\mu, \widehat{\mu}) \;:=\; \inf_{X\sim\mu,\ \widehat{X}\sim\widehat{\mu}} \mathsf{E}\left[\|X - \widehat{X}\|^p\right]^{1/p}, \qquad p \geq 1.$$

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- W_2-distance of Gaussian measures explicitly known [Gelbrich, 1990],

$$\mathsf{W}_2\left(\mathsf{N}(m, C), \mathsf{N}(\widehat{m}, \widehat{C})\right)^2 = \|m - \widehat{m}\|^2 + \operatorname{tr} C + \operatorname{tr} \widehat{C} - 2\operatorname{tr}\left(\sqrt{C}\widehat{C}\sqrt{C}\right)^{1/2},$$

and, e.g., $\mathsf{W}_p\left(\mathsf{N}(m, \sigma^2 C), \mathsf{N}(m, \widehat{\sigma}^2 C)\right) \leq |\sigma - \widehat{\sigma}|$

Sensitivity in Wasserstein Distance

- [Ernst, Pichler, S., 2020]: If $S\colon \mathscr{A} \to \mathscr{U}$ is globally Lipschitz with Lipschitz constant Lip_S, then for any probability measures $\mu, \widehat{\mu}$ on $\mathscr{A}$ we have

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  Example: $\mu = \mathrm{N}(0,1)$, $\mu_\epsilon = \mathrm{N}(0, 1+\epsilon)$ and $S(x) := \mathrm{e}^x$, $x \in \mathbb{R}$, then

$$\frac{\mathrm{W}_p(S_*\mu, S_*\mu_\epsilon)}{\mathrm{W}_p(\mu, \mu_\epsilon)} \xrightarrow{\epsilon \to +\infty} +\infty$$

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Then for any $\mu, \widehat{\mu}$ with

$$\mathsf{E}_{\mu}\left[\mathsf{Lip}_S^{2p}(\|a\|_{\mathscr{A}})\right],\ \mathsf{E}_{\widehat{\mu}}\left[\mathsf{Lip}_S^{2p}(\|a\|_{\mathscr{A}})\right] \leq C < \infty$$

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Which measures $\mu, \widehat{\mu}$ satisfy the integrability assumption for $\mathrm{Lip}_S(r) \in \mathscr{O}(\mathrm{e}^{\beta r})$?

Special case: Gaussian random fields

- Recall Gaussian random fields $a \sim \mathsf{N}(m, c)$ with continuous mean function $m \in C(D)$, $D \subset \mathbb{R}^d$ compact, and Matérn covariance functions

$$c_{\sigma^2,\rho,k+\frac{1}{2}}(x,y) := \sigma^2 \mathrm{e}^{-\frac{\sqrt{2k+1}}{\rho}|x-y|} \frac{k!}{(2k)!} \sum_{i=0}^{k} \frac{(k+i)!}{i!(k-i)!} \left(2\frac{\sqrt{2k+1}}{\rho}|x-y| \right)^{k-i}$$

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- We consider the following **subclass $\mathscr{G}$ of Gaussian measures on $C(D)$**

$$\mathscr{G} = \mathscr{G}(\mathscr{M}, \mathscr{C}) := \{\mathsf{N}(m,c) \colon m \in \mathscr{M}, c \in \mathscr{C}\}$$

$$\mathscr{M} = \{m \colon \|m\|_{C(D)} \le r_{\mathscr{M}}\}$$

$$\mathscr{C} = \left\{c_{\sigma^2,\rho,k+\frac{1}{2}} : \sigma \le \sigma_{\max},\ \rho \ge \rho_{\min}, k \in \{0,\dots,k_{\max}\}\right\}$$

- [Ernst, Pichler, S., 2020]: By means of Fernique's theorem and Dudley's entropy bound we have

$$\sup_{\mu \in \mathscr{G}} \mathsf{E}_{\mu} \left[\exp \left(\beta \, \|a\|_{C(D)} \right) \right] < \infty, \qquad \beta > 0.$$

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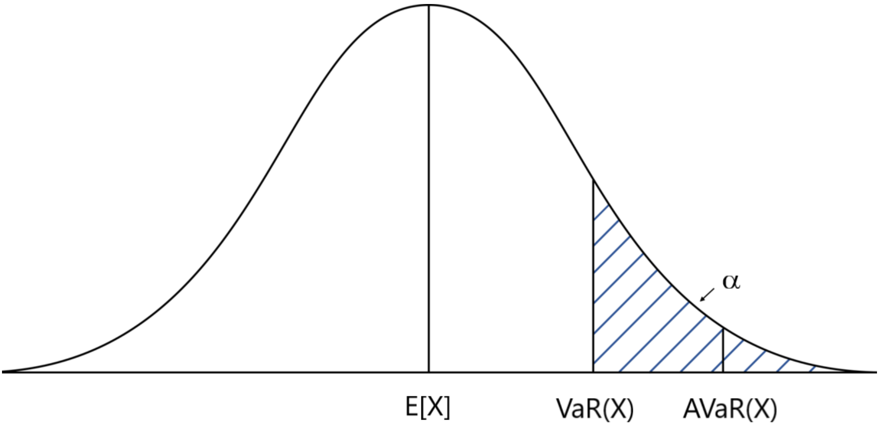
Risk Functionals – Illustration



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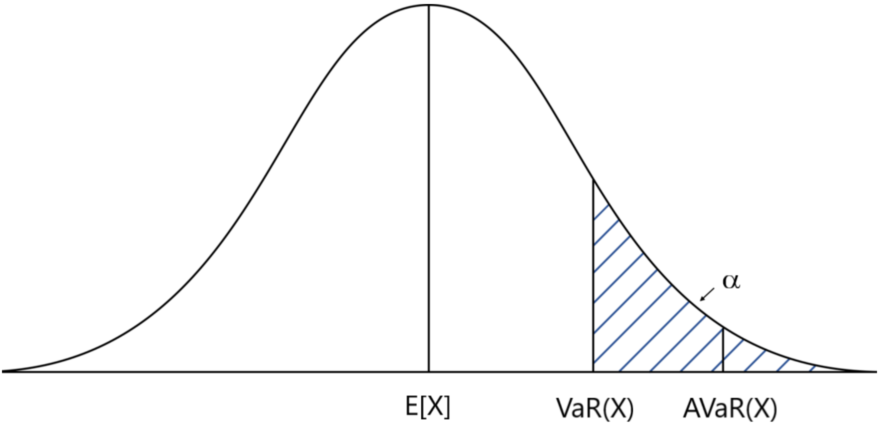

Goal

Control effect of underlying distribution $u \sim \nu$ on risk value $\mathrm{R}(q(u))$

Coherent Risk Functionals [Artzner et al., 1997]

- Common class of risk functionals which are
  1. **monotone:** $X \overset{\text{a.s.}}{\leq} Y \quad \Rightarrow \quad \mathsf{R}(X) \leq \mathsf{R}(Y)$
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Dual representation

By means of the Fenchel–Moreau theorem

$$\mathsf{R}(X) = \sup_{H \in \mathscr{H}} \mathsf{E}\,[H\ X]\,, \qquad \mathscr{H} \subseteq \{H \colon H \geq 0 \text{ a. s. and } \mathsf{E}\,[H] = 1\},$$

i.e., H basically represent probability density functions.

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where $u \sim \nu$ and $\widehat{u} \sim \widehat{\nu}$.

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for Hölder-continuous $q\colon H_0^1(D) \to \mathbb{R}$

Bayesian Inverse Problems (BIP)

- **UQ approach to inverse problem**

$$y = G(a) + \varepsilon, \qquad G \colon \mathscr{A} \to \mathbb{R}^k, \qquad \varepsilon \sim \mathsf{N}(0, \Sigma),$$

e.g., $G = O \circ S$ with observational map $O \colon \mathscr{U} \to \mathbb{R}^k$ applied to $u = S(a)$

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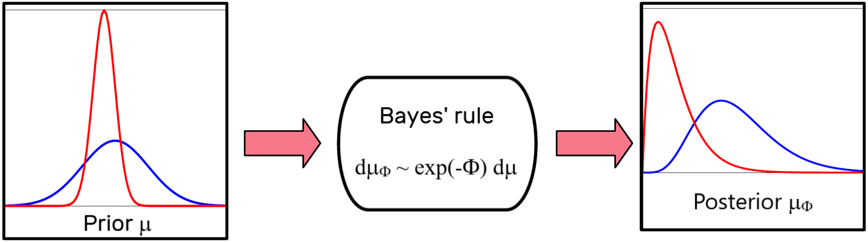
- **Question:** How sensitively depends μ_Φ on (subjective) choice of μ ?

Sensitivity of Bayesian Inversion



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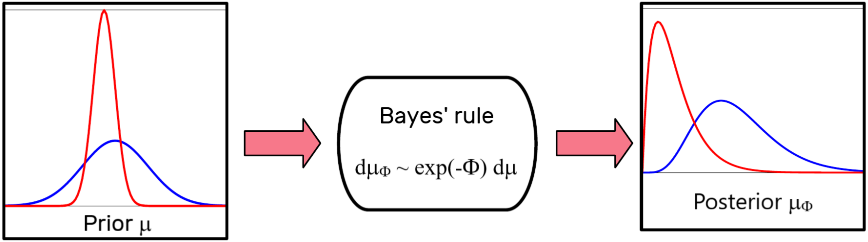

Theorem (informal, [S., 2020])

For d being TV, Hellinger, or 1-Wasserstein distance or KL divergence we have under suitable assumptions a locally Lipschitz continuity:

$$d(\mu_\Phi, \widehat{\mu}_\Phi) \;\leq\; C_\Phi(r)\; d(\mu, \widehat{\mu}), \qquad \text{if} \;\; d(\mu, \widehat{\mu}) \leq r$$

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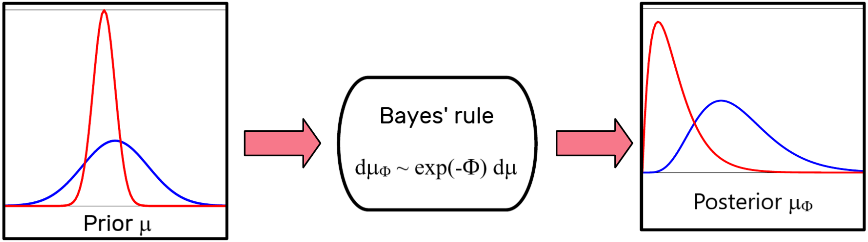

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But: $C_\Phi(r) \to \infty$ as data y more informative, e.g., noise $\varepsilon \to 0$

Wasserstein Distance

Theorem

1. If $\Phi\colon \mathscr{A} \to \mathbb{R}_+$ is continuous, we have continuity in p-Wasserstein distance, i.e.,

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Remark: [Diaconis & Freedman, 1986] studied Fréchet derivative $\partial T_\Phi(\mu)$ of mapping $T_\Phi(\mu) := \mu_\Phi$ w.r.t. TV distance topology and obtained

$$\|\partial T_\Phi(\mu)\| \simeq \frac{1}{Z}$$

Summary

- Locally Lipschitz sensitivity of uncertainty propagation w.r.t. Wasserstein distance for locally Lipschitz forward maps
- Also locally Hölder sensitivity of risk functionals for Hölder-continuous quantities of interest
- Similar results for sensitivity of Bayesian inversion w.r.t. choice of prior (or perturbations of log-Likelihood Φ)

More information:

[1] O. Ernst, A. Pichler, B. Sprungk. Sensitivity of Uncertainty Propagation for the Elliptic Diffusion Equation. *SIAM/ASA Journal on Uncertainty Quantification* (to appear), 2022.

[2] B. Sprungk. On the local Lipschitz stability of Bayesian inverse problems. *Inverse Problems* **36**, 2020.